

Phase Behaviour of the System (Carbon Dioxide + *n*-Heptane + Methylbenzene) and (Carbon Dioxide + Methane + Methylbenzene): a Comparison between Experimental Data and SAFT- γ -Mie Predictions

Saif Al Ghafri^{C, S}, J.P. Martin Trusler, Amparo Galindo, George Jackson and Geoffrey C. Maitland
*Qatar Carbonates and Carbon Storage Research Centre (QCCSRC), Molecular Systems Engineering,
Department of Chemical Engineering, Imperial College London, London, United Kingdom
sa1806@ic.ac.uk*

Simon Dufal
Department of Chemical Engineering, Imperial College London, London, United Kingdom

In this work, a new experimental apparatus was designed and constructed to measure the phase equilibria in systems containing CO₂ and hydrocarbons at reservoir temperatures and pressures. The apparatus involved a high-pressure high-temperature variable-volume view cell driven by a computer-controlled servo motor system. The maximum operating pressure and temperature were 40 MPa and 473.15 K, respectively. The apparatus was calibrated and validated by comparison with published isothermal vapour-liquid equilibrium data for the different binary systems. The vapour-liquid phase behaviour of the mixture (CO₂ + *n*-heptane + methylbenzene) was measured over the temperature range (298 and 473) K and pressures up to 16 MPa. The molar ratio between *n*-heptane and methylbenzene in the ternary system was fixed at different values, and the bubble-curve and part of the dew-curve was measured under carbon dioxide addition along five isotherms. The ternary mixture (CO₂ + methane + methylbenzene) was measured over the temperature range (323 and 473) K and pressures up to 36 MPa. The molar ratio between CO₂ and methane in the ternary system was fixed at different values (0, 0.25, 0.5, 0.75 and 1), and the bubble-curve and part of the dew-curve was measured under carbon dioxide addition along four isotherms.

In this work, we explore the predictive capability of SAFT- γ -Mie [1] to model the phase equilibria of the ternary mixtures. The Statistical Associating Fluid Theory, stemming from the first order perturbation theory of Wertheim [2], was implemented in this work with a group contribution approach and the generalized Mie potential to represent segment-segment interactions. In the resulting SAFT- γ -Mie, complex molecules are represented by fused segments representing the functional groups from which the molecule may be assembled. All interactions, both like and unlike, as implemented in this work were determined from experimental data of systems comprising the constituent groups.

References

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